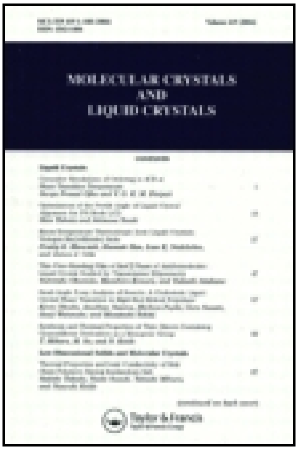

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The "Accurate" Separation of the Composite Thermally Stimulated Current Curves… From the Clear Standard to the Realistic Standard…

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THE "ACCURATE" SEPARATION OF THE COMPOSITE THERMALLY STIMULATED CURRENT CURVES
··· FROM THE CLEAR STANDARD TO THE REALISTIC STANDARD ···

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Abstract To accurately separate the composite thermally stimulated current curve into single curves, the original concept of the fundamental element is indispensable. To accurately establish the peak coordinate as the clear standard leads to utilizing substantial quantities.

INTRODUCTION

Presently, fundamental studies from various points of view are demanded to utilize various organic substances as available new materials. The thermally stimulated current (TSC) methods[1] have been widely utilized to study such fundamental characteristics in organic materials. The electronic states of organic substances are usually quite narrow[2,3], and then it was confirmed that the carrier-trap states were discretely distributed and each of them could be explained by the TSC curve of the first order[4]. In this paper, it is reported that the "accurate" separation of composite TSC curves is possible by the new TSC theory after measurement.

THEORY

The new TSC curve[5] which makes it possible to establish an accurate TSC curve has been already proposed from the original concept of the fundamental element. The fundamental equation of the first-order TSC curve of the slow retrapping model with constant heating rate is given as follows,

$$I = I_0' \cdot \nu \cdot \exp\left[-\frac{E_t}{kT} - \frac{\nu}{\beta}\int_{T_0}^{T} \exp\left(-\frac{E_t}{kT}\right) \mathrm{d}T\right] \quad (1)$$

Here, E_t: the energy depth of carrier trap (eV), ν: an escape frequency factor (1/s), β: the heating rate (K/s).

The fundamental equation of the proposed new TSC curve is given as

$$A=E_t\cdot B\ , \qquad (2)$$

$$A=-(\ln I-\ln I_P)+\sum_{n=0}(-1)^n\cdot\frac{(n+1)!}{A^n}\cdot\left(\frac{T_P-T}{T}\right)^n\cdot\left[1-\left(\frac{T}{T_P}\right)^{n+2}\cdot e^{-A}\right], \qquad (3)$$

$$B=\frac{1}{kT}-\frac{1}{kT_P}\ . \qquad (4)$$

It is important in the later discussions that parameters A and B were defined with no approximations and by which the proposed new TSC curve takes the shape of <u>a straight line passing through the origin</u>. The slope of the new TSC curve gives the accurate value of E_t; the intrinsic parameter of carrier trap. A representative of the first-order TSC curve and the corresponding new TSC curve are illustrated in Figs. 1 and 2. The peak coordinate point ③ is equivalent to the origin in Fig. 2, and the signs in both curves show the correct one-to-one correspondence.

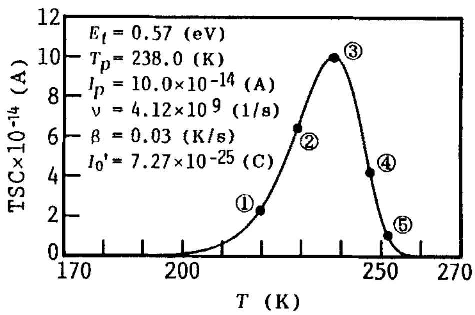

FIGURE 1　An example of the usual TSC curve.

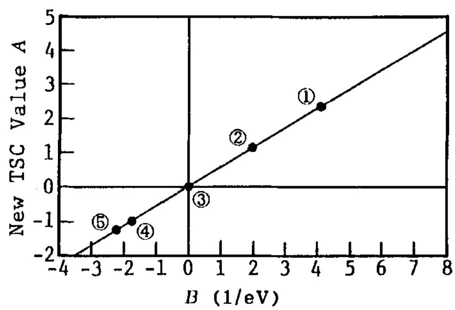

FIGURE 2　The new TSC curve.

<u>Recognition and Characteristics of the New TSC Curve</u>

In Fig. 3, the first-order TSC curve and two straight lines are illustrated on the defined coordinates of the Boltzmann function. In the new TSC curve theory, the peak point is rigidly recognized from the original concept of the fundamental element as the clear point exposing the physical balance between the contribution from detrapping and that from detrapped sites. The defined parameters A and B are fully recognized as the correct differences from this clear standard point. Additionally, point e can be translated from point d with no mathematical error. Therefore, the proposed new TSC curve can ideally establish a straight line passing through the origin on the defined A-B coordinates. Figure 3 is floating characteristic; the axis has no clear

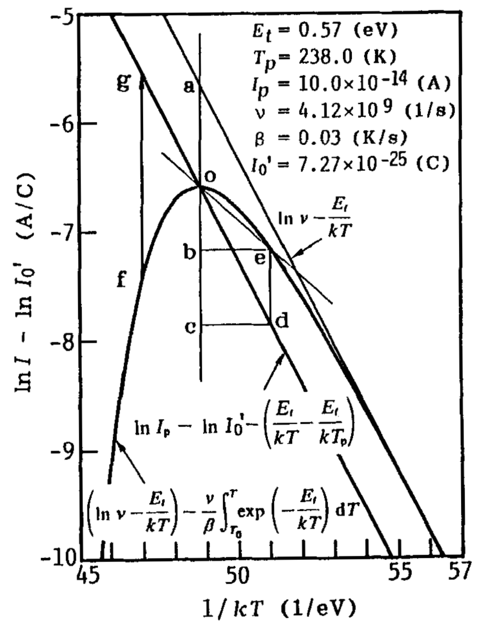

FIGURE 3 The TSC curve and two linear functions by which to recognize the physical meaning of the new TSC curve.

standard as the zero level. However, it is very important that the shape revealed on the coordinates of the Boltzmann function is uniformly fixed if the intrinsic parameter E_t value was unchanged. In other words, it was made clear for the first time that the shape was not influenced by experimental conditions at all. As the another intrinsic parameter ν also determines the position of the longitudinal axis in Fig.3, the fundamental equation of the first-order TSC curve was shown as eq.1.

The theory of the new TSC curve was completed on the basis of the concept of the fundamental element. A new TSC curve is comprised from the substantial organization of the substantial fundamental elements. Each of the fundamental elements which can freely be determined on the objective TSC curve is surely supported by the clear standard; the concept of the center. In other words, each of the fundamental elements of the new TSC curve should individually be supported by the original concept of the one-to-one relation; i.e., each fundamental element should individually be referred to the clear standard. Only reorganization of the substantial fundamental elements which have accurately been established by the accurate clear standard can obtain a straight line passing through the origin; i.e., an ideal figure. That is, an ideal figure reflects the rigid case. Then, this ideal straight line can be utilized as the realistic standard in the "accurate" separation of the composite TSC curves as described later.

If the peak coordinate point used as the only clear standard point had a little uncertainty, the new TSC curve would deviate from the straight line. In the new TSC theory, however, the organization of the translated fundamental elements makes it possible to independently recorrect the values of the peak coordinates. That is, self-cleaning operation is possible. And these are the fine characteristics which only the new TSC theory proposed on the concept of the fundamental element possesses.

ACCURATE SEPARATION OF THE COMPOSITE TSC CURVES

In Figs. 4, 5, an example of the composite TSC curve and the corresponding new TSC curve are illustrated. In this case, accurate separation is possible by utilizing only the lower temperature region than the apparent peak point. This simulation case corresponds to the well-found experimental data. Because discussions about the separation of composite curves should also be started from the case contributed only by two carrier traps.

Generally, it is well known that the electronic states are quite narrow; i.e., ca. 0.015 eV[2] and 0.01-0.05 eV[3]. Thus, the carrier trapped in organic substances also can naturally be deduced to be existed in such narrow states. From these consideration, an example in which two carrier traps are neighbor has been simulated from considering the experimental data in anthracene single crystals; electron traps of 0.12 and 0.15 eV. If the state-width were ca. 0.01 eV, this case corresponds to the energy gap of ca. 0.01 eV.

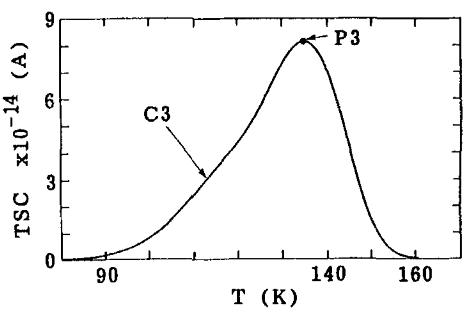

FIGURE 4 An example of the composite TSC curve.

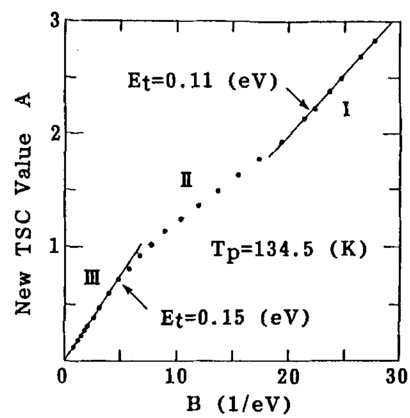

FIGURE 5 The new TSC curve corresponding to Fig. 4.

In Fig.5, the apparent values which were read out from the peak coordinate in Fig.4 are used to calculate the new TSC curve. In Fig.4, it is not clear to detect whether or not the objective curve is single. On the other hand, figure 5 enables one to detect that the curve is surely comprised by two carrier traps; i.e., the composite case. Two straight regions can be found, i.e., the region III near the origin and the region I far from the origin. Therefore, it can clearly be deduced that the main curve has the some contribution from another carrier trap in the lower temperature region. Such sure detection is very important as the first step of the accurate separation. The actual processes of accurate separation are explained as follows.

1) The TSC curve C2 is calculated from the slope of the region III, and is subtracted from the whole curve shown in Fig.4 on the zero base axis.

2) The concealed C1 curve, which is illustrated in Fig.6, is exposed for the first time. In the following steps, it becomes key processes to establish a single curve by utilizing the new TSC theory availably.

3) The peak coordinates (T_p, I_p) of this exposed TSC curve are not usually accurate. This can easily be detected because the new TSC curve of C1 does not pass the origin in Fig.7. And the values of the peak coordinate should rigidly be refined to an ideal case because the peak coordinate is <u>the clear standard</u>. Simultaneously, each fundamental element can surely be refined. In this example, only the T_p value was recorrected from 112.5 to 112.8 (K).

4) The refined C2 curve also should be exposed from this refined C1 curve from subtraction on the zero coordinate.

In each step, it should be confirmed whether or not the exposed TSC curves are fully accurate. Generally, the mutual revision should alternately be repeated. These are the fine characteristics of the proposal; the self-convergence.

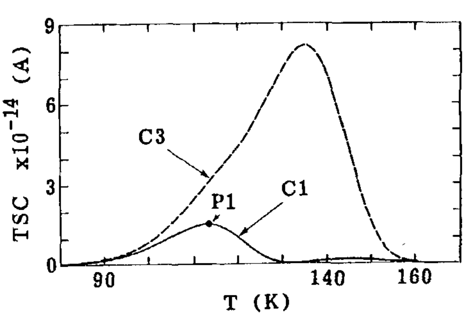

FIGURE 6 An exposed C1 curve.

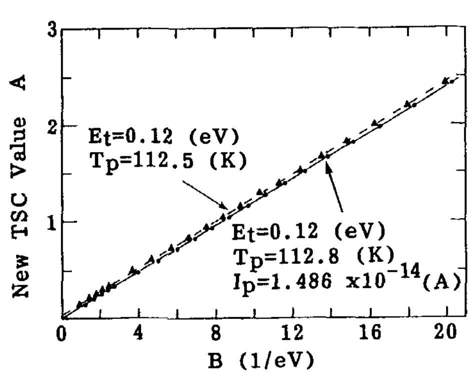

FIGURE 7 The new TSC curve corresponding to Fig.6.

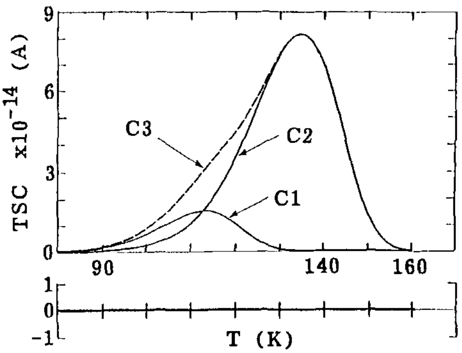

FIGURE 8 Two curves finally established.

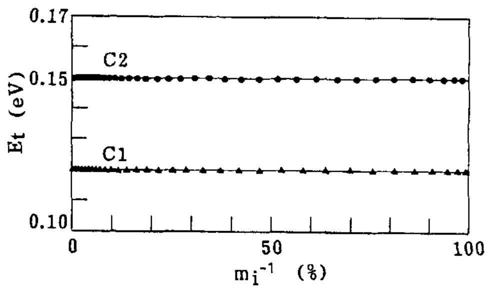

FIGURE 9 The m-characteristics and "accuracy".

5) Two curves finally established are illustrated in Fig.8. In other words, substantial reorganization of the substantial fundamental elements is individually confirmed. In Fig.9, "accuracy" of the established TSC curves is severally confirmed by the m-characteristic of the asymptotic estimation L-method[6]. The flatness verifies the accuracy of the TSC curve in fine detail.

CONCLUSION

From detailed discussion as described above, it has made clear that accurate separation of the composite TSC curve starts from the clear detection whether or not the objective is single, successively finishes after the accurate establishment of the single curves which were exposed from the composite TSC curve. There, recognition of the clear standard, the one-to-one relation and the realistic standard were indispensable and establishment of the substantial quantities enabled us to originally express "accuracy" in details.

This proposal is not only to discuss accurate separation but also will make it possible to discuss the electronic states in organic substances in fine detail in the near future.

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